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On the evaluation of the trapping parameters from thermoluminescence glow curves

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Abstract : A critical appraisal of a method of determination of trapping parameters associated with thermoluminescence glow curves proposed by Vejnovic *et al* has been made. It is concluded that contrary to their claim their method is not superior to the method of determination of trapping parameters using peak widths.

Keywords : Thermoluminescence, order of kinetics, activation energy, frequency factor, symmetry factor.

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1. Introduction

The determination of trapping parameters from thermoluminescence (TL) glow curves is an active area of interest and various techniques have been developed for the determination of trapping parameters namely activation energy (E), order of kinetics (b) and frequency factor (s) in kinetics formalism [1–4]. Analysis of TL has become more important in view of its applications in dating, dosimetry and defect studies. The kinetics formalism in spite of its limitations is still useful in the analysis of TL [5].

Recently Vejnovic *et al* [6] have proposed a new method of determination of trapping parameters and claimed that their method is more rigorous than the conventional peak shape methods [1,2]. They have failed to note that the non-uniqueness of the symmetry factor (μ_g) for a particular order of kinetics in the case of TL recorded with linear heating scheme was pointed out long ago independently by Gartia *et al* [7] and Hoogenboom *et al* [8]. Based on the works of Gartia *et al* [7,9], Singh *et al* [10] proposed a method of determination of TL parameters by using peak widths. Similarly Singh *et al* [11] have developed a method of determination of trapping parameters for TL recorded in a hyperbolic heating scheme. In the present article we critically examine the method of Vejnovic *et al* [6] by considering both numerically computed and experimental TL peaks. We also consider the method of Singh *et al* [10] for TL recorded in hyperbolic heating scheme.

2. Theory

Following Singh *et al* [10] the mean symmetry factor (μ_g) of a general order TL peak recorded in a linear heating scheme can be expressed as

$$\mu_g = 0.2453 + 0.1858b - 0.0244b^2. \tag{1}$$

Now if T_1 and T_2 are half intensity temperatures we can write [1–3]

$$\mu_g = \frac{T_2 - T_m}{T_2 - T_1} \tag{2}$$

where T_m is the peak temperature. For the TL peak under consideration, knowing μ_g from equation (2) order of kinetics can be determined from equation (1). Activation energy can be obtained from the relations

$$E_\tau = C_\tau kT_m^2/\tau + D_\tau kT_m \tag{3}$$

$$E_\delta = C_\delta kT_m^2/\delta + D_\delta kT_m \tag{4}$$

$$E_\omega = C_\omega kT_m^2/\omega + D_\omega kT_m \tag{5}$$

where $\tau = T_m - T_1$, $\delta = T_2 - T_m$, $\omega = T_2 - T_1$ and k is the Boltzmann constant. From (2) one can write

$$\mu_g = \frac{\delta}{\omega} \tag{6}$$

The coefficients C_j and D_j can be expressed as a quadratic function of b [10]

$$C_j = C_{0j} + C_{1j}b + C_{2j}b^2 \tag{7}$$

$$D_j = D_{0j} + D_{1j}b + D_{2j}b^2 \tag{8}$$

The coefficients C_{kj} and D_{kj} ($k = 0$–$2, j = \tau, \delta, \omega$) have been reported by Singh *et al* [10]. Finally the frequency factor can be obtained as

$$s = \beta \Big/ \left\{ \frac{bkT_m^2}{E_{av}} \exp\left(-E_{av}/kT_m\right) - (b-1)\int_{T_0}^{T_m} \exp\left(-E_{av}/kT\right) dT \right\} \tag{9}$$

where β is the heating rate, T_0 is the initial temperature and E_{av} is the average of E_τ, E_δ and E_ω.

Although for experimental convenience TL is normally recorded with a linear heating programme the hyperbolic or reciprocal heating scheme can be considered as an important adjunct to the traditional linear heating profile and it can be used for cross checking the values of trapping parameters obtained by using the conventional linear heating scheme as done by Bos *et al* [12] for the case of LiF : MgTi (TLD-100).

The hyperbolic heating scheme can be expressed as [10]

$$\frac{1}{T} = \frac{1}{T_0} - \beta' t \tag{10}$$

where T is the temperature at time t and β' is a constant. The heating rate corresponding to the peak temperature T_m is given by

$$\beta_m = \beta' T_m^2 \tag{11}$$

For hyperbolic heating scheme the symmetry factor can be expressed as [13]

$$\mu_g = \frac{(1/T_m) - (1/T_2)}{(1/T_1) - (1/T_2)}. \tag{12}$$

It may be noted that this particular point has been overlooked by Vejnovic *et al* [6]. As shown by Singh *et al* [11]

$$\mu_g = 0.2716 + 0.1543b - 0.0200b^2 \tag{13}$$

In the case of hyperbolic heating scheme for a particular b E_τ, E_δ and E_ω can be determined from equations (3–5), but the coefficients C_{kj} and D_{kj} ($k = 0$–$2, j = \tau, \delta, \omega$) are different from those for linear heating scheme. The corresponding coefficients for hyperbolic heating profile have been presented by Singh *et al* [11]. The frequency factor can be obtained from the equation

$$\frac{sk}{\beta' E} = \left[\exp(-E/kT_m) + (b-1)\exp(-E/kT_0)\right]^{-1} \tag{14}$$

3. Results and discussions

We have followed the numerical technique outlined by Singh *et al* [10]. The only difference lies in the evaluation of second exponential integral $E_2(x)$ [14] which arises in connection with the evaluation of the integral occurring in the expressions for TL intensity [10]. Following the works of Gartia *et al* [7] and Mazumdar *et al* [15] Singh *et al* [10] has used a rational approximation for the evaluation of $E_2(x)$. In the present paper we evaluate $E_2(x)$ following a rigorous method developed by Devi [16] who has used a continued fraction representation of $E_2(x)$.

As a check of the computer code we have evaluated μ_g of the computer generated TL peaks used by Vejnovic *et al* [6] which incidentally are identical to those used by Chen [17]. The present μ_g values although in agreement with those of Chen are somewhat different from those of Vejnovic *et al*. In view of this in Table 1 we recompute the values of trapping parameters E_v, b_v and s_v corresponding to the method of Vejnovic *et al* by using

Table 1. Trapping parameters of some computer generated TL peaks calculated by the method of Vejnovic *et al* [6]. All peaks correspond to a linear heating rate of 0.5 K/s.

Sl. No.	E (eV)	b	s (sec^{-1})	μ_g[6]	μ_g[10]	E_v (eV)	b_v	s_v (sec^{-1})
1	1.6	2.5	10^{13}	0.572	0.548	1.75	2.75	2.6×10^{14}
2	1.6	1.9	10^{13}	0.518	0.509	1.79	1.85	6.36×10^{14}
3	0.4	1.5	10^{13}	0.470	0.476	0.459	1.57	1.32×10^{15}
4	1.6	1.5	10^9	0.478	0.481	1.83	1.56	4.13×10^{10}
5	0.4	1.5	10^9	0.480	0.482	0.457	1.56	3.35×10^{10}
6	0.1	1.5	10^9	0.482	0.483	0.114	1.55	2.71×10^{10}
7	0.1	0.7	10^8	0.316	0.372	0.123	0.887	1.23×10^{10}
8	1.6	0.7	10^5	0.336	0.376	1.96	0.882	4.66×10^6
9	0.4	1.9	10^5	0.545	0.526	0.439	1.77	4.85×10^5
10	0.1	1.9	10^5	0.549	0.528	0.109	1.75	3.92×10^5
11	0.1	2.5	10^5	0.604	0.565	0.106	2.08	2.43×10^5

the present μ_g values. The T_m values reported by them are also marginally different from the present values because they use an approximate equation [equation (5) of their paper for the calculation of T_m]. In Table 2 we present the trapping parameters E_p, b_p and s_p for the same set of computer generated peaks by using the method of Singh *et al*. A close inspection of Tables 1 and 2 reveal that contrary to the claim of Vejnovic *et al* [6] the values of the trapping parameters as calculated by the method of Singh *et al* are marginally better than those of Vejnovic *et al* [6] when comparisons are made with their input values.

In Table 3 we present the values of trapping parameters of earlier set of computer generated TL peaks recorded in a hyperbolic heating scheme corresponding to the heating rate of 0.5 K/s at peak temperature. Here the values of E_p, b_p and s_p are in better agreement with the input values of trapping parameters than in the case of linear heating scheme because here μ_g is a unique function of order of kinetics.

Table 2. Trapping parameters of some computer generated TL peaks calculated by the method of Singh *et al* [10]. All peaks correspond to a linear heating rate of 0.5 K/s.

Sl. No	E (eV)	b	s (sec^{-1})	μ_g[6]	μ_g[10]	E_p (eV)	b_p	s_p (sec^{-1})
1	1.6	2.5	10^{13}	0.572	0.548	1.55	2.35	3.39×10^{12}
2	1.6	1.9	10^{13}	0.518	0.509	1 60	1.89	$9\ 77 \times 10^{12}$
3	0.4	1.5	10^{13}	0 470	0.476	0.409	1.56	2.17×10^{13}
4	1.6	1.5	10^{9}	0 478	0.481	1.66	1.61	2.64×10^{9}
5	0.4	1.5	10^{9}	0 480	0.482	0.416	1.62	2.73×10^{9}
6	0.1	1.5	10^{9}	0.482	0.483	0.104	1.63	$2\ 82 \times 10^{9}$
7	0.1	0.7	10^{8}	0.316	0 372	0 104	0 753	2.51×10^{8}
8	1.6	0.7	10^{5}	0.336	0 376	1.70	0.782	$2\ 95 \times 10^{5}$
9	0.4	1.9	10^{5}	0 545	0 526	0 419	2.08	2.16×10^{5}
10	0.1	1.9	10^{5}	0.549	0.528	0.105	2.11	$2\ 24 \times 10^{5}$
11	0.1	2.5	10^{5}	0.604	0.565	0.102	2.63	1.33×10^{5}

Table 3. Trapping parameters of some computer generated TL peaks recorded in a hyperbolic heating scheme. Heating rate at peak temperature is 0.5 K/s.

Sl. No.	E (eV)	b	s (sec^{-1})	μ_g[13]	E_p (eV)	b_p	s_p (sec^{-1})
1	1.6	2.5	10^{13}	0.531	1.60	2.48	$9\ 92 \times 10^{12}$
2	1.6	1.9	10^{13}	0.493	1 60	1 90	9.71×10^{12}
3	0.4	1.5	10^{13}	0 460	0.399	1.52	9.57×10^{12}
4	1.6	1.5	10^{9}	0.460	1.60	1.52	9.65×10^{8}
5	0.4	1.5	10^{9}	0.460	0.399	1.52	9.66×10^{8}
6	0.1	1.5	10^{9}	0.460	0.100	1.52	9.67×10^{8}
7	0.4	1.9	10^{5}	0.493	0.399	1.90	9.64×10^{4}
8	0.1	1.9	10^{5}	0.493	0.100	1.90	9.61×10^{4}
9	0.1	2.5	10^{5}	0.531	0.100	2.48	9.55×10^{4}

Finally we consider some well analysed experimental [15,18,19] TL peaks namely 165.5°C TL peak of Ca doped KCl and 320°C peak of bluish green microclene. From Table 4 we observe that even for experimental TL peaks the values of trapping parameters as calculated by the method of Singh *et al* are in better agreement with those (E_{cf}, b_{cf}, s_{cf})

obtained by rigorous method of curve fitting when comparisons are made with the values of trapping parameters obtained by the method of Vejnovic *et al.*

Table 4. Trapping parameters of some experimental TL peaks.

Trapping parameters	165.6°C TL peak of Ca doped KCl	320°C TL peak of Bluish green microclene
E_{cf} (eV)	1.36	1.42
E_p (eV)	1.40	1.42
E_v (eV)	1.63	1.58
b_{cf}	1.0	2.0
b_p	1.1	2.0
b_v	1.2	1.9
s_{cf} (sec^{-1})	1.46×10^{14}	3.44×10^{10}
s_p (sec^{-1})	4.93×10^{14}	3.75×10^{10}
s_v (sec^{-1})	2.18×10^{17}	9.18×10^{11}

4. Conclusion

We have critically examined a method of calculation of TL trapping parameters recently proposed by Vejnovic *et al* and observe that their method does not lead to the improvement of accuracy of calculation of trapping parameters by applying their method both to computer generated and experimental TL peaks and by comparing the trapping parameters so obtained with those evaluated by using a method proposed by Singh *et al* [10].

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